CINT User Capabilities

Revised: April 15, 2009

CINT capabilities are provided to users through the CINT Scientists and other technical contacts. Listed below are brief descriptions of these capabilities and the associated staff who use them for their nanoscience integration research. In some cases, one capability may be used by several staff members in distinct ways; hence we provide multiple contact names in order that the prospective user may determine the appropriate staff member through which the capability may be accessed.

We strongly encourage prospective CINT users to contact the person(s) associated with a capability of interest in order ensure that the capability will meet the needs of the user. We welcome user proposals that involve multiple capabilities.

CINT has made arrangements for CINT users to also access other National User Facilities at Los Alamos National Laboratory and Sandia National Laboratories. Prospective users whose research would require capabilities at CINT and these other User Facilities can submit one proposal to access the combined facilities.

I. Experimental Capabilities: *Synthesis and Fabrication*

Physical synthesis of nanostructured materials

Our physical vapor deposition (PVD) capabilities are used to synthesize metal, alloy, ceramic or composite materials where the internal nanostructuring dimension such as layer thickness, grain size or particle size may be well controlled down to the nanometer level. Some examples include, but are not limited to, nanolayered composites, metals or alloys with nanometer-scale grain size, crystalline or amorphous matrixes embedded with nano-dots with well-controlled sizes and spacing, nano-twinned materials, etc. The total thickness of the sample may vary from sub-micrometer to a few tens of micrometers. Through appropriate masking techniques, the films could be pattern in shapes, e.g., as self-supported tensile samples. Energetic ion or neutral atom bombardment during growth are used to tailor the nanostructuring dimension, residual stress, texture, epitaxy, etc. Post-deposition vacuum annealing or ion-bombardment facilities are also available for modification of the PVD-synthesized materials. Collaborative work on stresses and mechanical behavior, physical properties such as magnetic, electronic and optical, thermal properties, fatigue, thermal stability, fracture, and creep of these PVD-synthesized nano-materials as a function of the nanostructuring dimensions is envisioned.

Capabilities available include:

- Electron beam evaporation
- Magnetron sputtering

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III-V Semiconductor molecular beam epitaxy

The molecular beam epitaxy (MBE) capabilities allow the growth of As-based III-V compound semiconductors. The system specializes in high-purity, high-mobility materials grown with monolayer precision. Due to the high-mobility nature of the system, only n-type doping using Si is available. Areas of interest for growth available to CINT Users include:

- Low dimension semiconductor systems
- Quantum transport
- Electronic devices based on intrasubband transitions.

Associated CINT Scientist:
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Semiconductor nanowire synthesis
Our low pressure chemical vapor deposition (CVD) system allows the synthesis of semiconductor nanowires based on the vapor-liquid-solid (VLS) technique. Currently this capability is focused on silicon and germanium nanowire growth using silane and germane along with p- and n-type electrical doping during growth using B and P precursor sources. Deposited metal nanodots such as Au are used to seed VLS growth. Areas of capability development and particular interest include:

- VLS growth of Si and Ge nanowires and growth kinetics studies
- Synthesis and properties of electrically doped Si and Ge nanowires
- Synthesis and properties of Si/Ge linear and core/shell heterostructures

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Epitaxial and nano-composite metal-oxide films
Wide use of metal-oxide materials in future device applications is expected due to the tremendous variety of phenomena that they exhibit such as high-temperature superconductivity, ferroelectricity, piezoelectricity, ferromagnetism, and semiconductive properties. Our pulsed laser deposition (PLD) and polymer-assisted deposition (PAD) capabilities allow one to deposit epitaxial and nano-composite metal-oxide films with superior properties over many conventionally utilized materials in terms of functionalities. The PLD and PAD also allow one to grow multilayer films for monolithic integration of dissimilar materials with complementary functionalities on a single platform to fabricate novel devices. Collaborations are welcome to explore new functional metal-oxide films, investigate the effects of strain imposed by coherent epitaxy on the properties of the films, and study nano-composite and multilayer metal-oxide films. Capabilities available include:

- Pulsed laser deposition
- Polymer-assisted deposition
- Ion-milling

Associated CINT Scientist:
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Micro- / nano- fabrication
The fabrication capabilities provide researchers with distinctive platforms for investigating standard or hybrid materials. Our 100 mm facility has an unrestricted tool set, which accommodates a wide range of substrates, films, and chemicals. We work closely with other centers/laboratories to allow integration of unique materials or processes into prototype micro/nano systems. The capabilities that are available to CINT Users include:

Fabrication capabilities:

- Contact mask photo-lithography (265 nm DUV, 365/400 nm NUV)
- Contact mask design and fabrication – 0.6 um resolution, 4", 5" or 7" substrates
- Metal deposition (E-beam and thermal evaporation)
- Dielectric thin film deposition (ICP CVD H-aSi, Si_3N_4, SiO_2, SiON)
- Reactive ion etching with laser endpoint detection (ICP and RIE fluorine; ICP chlorine; silicon deep RIE)
- Downstream Microwave Source plasma ash
- Rapid Thermal Annealing (up to 1000°C)
- Plasma and UV/Ozone cleaning
- Wet chemistries
- Wafer dicing and lapping (late 2009)
- Focused ion beam
- Electron beam lithography
- Laser beam direct write
- In-situ SEM mechanical nanoprobe
- Critical Point Dryer

Inspection capabilities:

- SEM / EDAX
- Pd/Au PVD for sample preparation

- Optical Microscope
- Confocal microscope
- Profilometer
- Probe-station
- Flexus Stress Measurement
- Ellipsometer
- Spectroscopic Reflectometer
- Four Point Resistivity Probe

Technical Contact:
John Nogan, jnogan@sandia.gov, (505) 284-8863

Electron beam lithography
The JEOL JBX-5FE Electron Beam Lithography System is a field-emission system operating at 50kV with a five inch stage. The minimum spot size is 5 nm and the minimum achievable feature size is on the order of 20 nm. Typical feature sizes are in the range of 50-250 nm. This instrument, in association with etch and deposition capabilities, provides powerful nanofabrication capabilities for a wide variety of materials and applications. Relevant parameters include:

- Can handle nominally rectangular samples in the range of 5-25 mm;
- Can handle wafers of 2, 3, 4, and 6 inches in diameter
- Typical positive resist used is PMMA
- Typical negative resist is SAL-603 or NEB-31A

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MEMS and NEMS fabrication and characterization
The MEMS/NEMS fabrication and characterization capability enables the creation of micromechanical and nanomechanical structures that are used to understand phenomena associated with the motion, displacement, or vibration of structures. Some research activities supported by this capability include studies of the size-, geometry-, material-, surface-, and temperature-dependence of mechanical dissipation in MEMS/NEMS resonators, studies of the mechanical properties and of mechanical deformation and fracture in thin film materials, studies of chemical, biological, or environmental sensing using mechanical structures, studies of phonon transport in geometrically-confined structures, and the development of new mechanical structures, such as custom cantilevers, for scanning probe microscopy. The following capabilities will be available:

- MEMS and NEMS surface micromachining, including contact mask and e-beam lithographic patterning , dry etching, and wet release.
- Laser light scattering in vacuum for detection of MEMS resonator motion, resonance frequency, and quality factor.
- Ultra-high vacuum, variable temperature AFM/STM for mechanical probing and scanning probe tip development and testing.

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Soft Nanolithography
Soft nanolithography refers to a group of patterning techniques that complement UV and electron beam lithography. These approaches bypass the harsh chemical and radiation exposure often used in conventional lithography processing, making them particularly useful for bio, organic, and molecular materials. For many of these techniques, an elastomeric stamp (typically made of polydimethylsiloxane, PDMS) with relief patterns is made from a “master” containing the complementary patterns. In micro-contact printing (μCP), the PDMS stamp is inked with molecules that form self-assembled monolayer (SAM) on the surface of interest. Stamping results in an organic template that consists of regions with different chemical properties and/or functionality. These templates can be used for etching or direct crystal growth, to name a few. In nano-transfer printing (nTP), a PDMS stamp is coated with a thin layer of metal, which can then be transferred onto surfaces to form metal patterns in an additive manner. Solution stamping nanolithography (SSNL) utilizes sol gel precursors as ink to form functional oxide patterns on a variety of surfaces without etching. We also have dip-pen nanolithography (DPN) capability that uses an atomic force microscope tip to

selectively deposit or remove organic molecules and sol precursors on surfaces. DPN enables us to extend the patterning feature size down to deep sub-micron regime. Capabilities available to CINT Users include:

- Micro-contact printing of SAMs on metal, oxide, semiconductor surfaces
- Nano-transfer printing of metal patterns on to hard and soft substrates
- Solution stamping nanolithography of functional oxide patterns on flat and curve surfaces
- Selective deposition of SAM molecules or sol precursors via dip pen nanolithography

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Polymeric monolayer systems
Surface properties are critical in many nanosystems, and the control of surface properties such as wetting, adhesion, and friction are of primary concern. Monolayer synthesis allows researcher to tailor surface properties utilizing small molecule organic synthesis and polymerization techniques. Either *in situ* or *ex situ* syntheses can be performed where appropriate and multilayers or gels may be produced using similar techniques. Capabilities that are available include:

- Monolayer design and formation on planar, particulate, chip-based, or other samples of inorganic oxides, non-oxidized metals, semiconductors, polymers, etc.
- Synthesis of functional coupling agents, in particular those with functionality.
- *In situ* modification of monolayer functionalities where desired functionalities lack compatibility.
- *In situ* growth of polymer monolayers and mixed polymer monolayers using free radical, ionic or coordination polymerization reactions.
- A suite of characterization methods to determine or verify monolayer functionality, structure, wetting properties, etc.

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Colloidal synthesis: Semiconductor, metal, and magnetic nanocrystals
In our laboratory we emphasize the preparation of "high-quality" semiconductor, metal, and magnetic nanocrystals. We define success in part by our ability to control size dispersity, particle crystallinity, particle stability, and particle optical/electronic/magnetic properties. These criteria comprise our definition of "high-quality." Typically, our nanocrystals are prepared with a target functionality in mind. We work closely with physicists and spectroscopists who, through their advanced characterization tools, inform our synthetic work. We strive to understand, for example, the effects of particle size, particle shape, and particle surface structure and functionalization on nanocrystal properties and, subsequently, to optimize these properties. We focus on the preparation of new compositions (core and core/shell materials; UV to visible to infrared absorbers/emitters; ferromagnetic to superparamagnetic nanoparticles, etc.), new shapes (isotropic to highly anisotropic), composite materials (*e.g.*, high-density nanocrystal/sol-gel processible blends), and biocompatible nanocrystals (water-soluble and functionalized for binding to various biomolecules), as well as self- and directed-assembly of films and composite structures. Nanocrystal chemical-precursor development and ligand/surfactant development are pursued when necessary. Capabilities available include:

- Facilities for synthesizing and assembling colloidal nanocrystals, and facilities for thin-film preparation, including air-sensitive handling methods, LB trough, and multi-gun sputtering system
- Expertise in inorganic, organic, and materials chemistry
- In-lab (and partner-lab) facilities for microstructural, optical and magnetic-properties characterization of nanoscale systems, including UV-Vis, near-IR FTIR, fluorimeter, AFM, NSOM, MFM, TEM, optical microscopy, and ultrafast laser spectroscopy

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Chemical synthesis of nanoscale electronic materials
Inorganic and organic synthetic chemical procedures leading to nanoscale electronic and optically active building blocks, including semiconductor quantum dots, metal nanoparticles and conjugated organic polymers are available. Capabilities include:

- Colloidal nanocrystal synthesis, as well as chemical-precursor and ligand development (see above)
- Synthesis of water soluble conjugated polymers

- Preparation of nanostructured fibers and composites, including chiral composites, involving conjugated polymers
- Synthesis and characterization of metal nanoparticles
- Stabilization of metal nanoparticles in solution

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Thin-film preparation
Preparation and characterization of thin-films using chemical assembly routes is possible for many different types of materials and substrates. The major focus of activities is on different self-assembly routes to thin-film materials, and on preparative strategies that involve combinations of processing (spin or dip-coating; post-deposition patterning) with self-assembly strategies. Specific capabilities available include:

- Dip-coating and spin coating of soluble polymers, including multi-layer assemblies of water soluble conjugated polymers and other poly-electrolytes;
- Langmuir-Blodgett capabilities, including multi-layer deposition and Brewster-angle microscopy characterization;
- Surface cleaning tools and techniques;
- Incorporation of nonlinear optical chromophores into amphiphilic assemblies and Langmuir-Blodgett films;
- Self-assembled monolayer formation on metal and oxide surfaces;
- Thin-films of mesoporous and mesostructured silica;
- Patterned films of electronically active nanoscale building blocks (conjugated polymers, fullerenes);
- Spatial patterning of organic thin films using masked deep-uv exposure

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Lipid membranes and self-assembled films
An assortment of capabilities exists for the synthetic preparation of functionalized amphiphiles and their incorporation in lipid vesicles, supported lipid membranes, self-assembled monolayers on silicon surfaces, and Langmuir films. The self-assembled films can be interrogated with a variety of spectroscopic techniques, which include dynamic light scattering, fluorescence microscopy and spectroscopy, NMR, and XPS, and at the nanoscale via *in situ* AFM imaging and TEM. Interactions of metal ions, small molecules, proteins, and whole cells against functionalized films have been previously explored. The capabilities that are available to CINT Users include:

- Wet laboratory facilities for the synthesis and characterization of functionalized amphiphilic molecules
- Liposome preparation via sonicators and extruders
- Langmuir troughs for monolayer and multilayer film preparation
- Inverted fluorescence microscope coupled with intensified CCD camera and CCD spectrometer for simultaneous imaging and spectroscopic characterization of Langmuir monolayers
- Temperature controlled *in situ* AFM for nanoscale imaging under varying environmental conditions
- Microcalorimetry to measure binding energies of protein association at lipid membrane surfaces
- Fluorescence recovery after photobleaching (FRAP) characterization of lateral mobility in substrate-supported lipid membrane assemblies
- Brewster angle microscopy for characterization of thin films
- Generation of patterned hybrid and supported bilayer assemblies on derivatized substrates
- Synthesis and assembly of lipids incorporating molecular recognition elements (peptides, chelates etc.)

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Mesoporous materials

Our work combines inorganic and hybrid (organic/inorganic) solution-based synthesis with molecular self-assembly to arrive at porous and composite nanostructured films and particles by simple evaporative procedures. Starting with homogeneous solutions of amphiphilic surfactants, lipids, or block copolymers, solvent evaporation drives the self-assembly of micelles and further self-organization into periodic mesophases, serving to organize added hydrophilic inorganic and/or hydrophobic organic precursors. Using such solutions as 'self-assembling inks', we print these periodic nanostructures onto arbitrary surfaces whose nano- micro- and macro-structures can be defined further with light. Replacing standard surfactant micelles with monosized nanocrystal micelles, we use evaporation-induced self-assembly to develop robust, patternable 3D arrays of metallic, semi-conductor or magnetic nanocrystals and to integrate them into devices or platforms, where they can be interrogated electronically, optically, or magnetically. Recently we discovered the ability of living cells to organize extended nanostructures and nano-objects in a manner that creates a unique, highly biocompatible nano//bio interface, mimicking the extra-cellular matrix. Using printing and patterning techniques, we can integrate cells into platforms needed for electronic, optical, and spectroscopic interrogation. Capabilities include:

- Evaporation induced self-assembly (EISA) of nanostructured membranes, porous electrodes, low *k* dielectric films on arbitrary surfaces
- Pore-gating with environmentally-actuated molecular valves
- Self-assembly and directed assembly of ordered organic/inorganic nanocomposite films
- Self-assembly and integration of 2- and 3-D nanocrystalline arrays
- Lithographic definition and patterning of nano-structured films
- Thermal and plasma-assisted atomic layer deposition of conformal oxides on nanostructures
- Aerosol-assisted self-assembly of controlled porous and composite nano-particles
- Cell-directed assembly of bio/nano interfaces – cell immobilization and patterning
- Sol-gel chemistry
- Superhydrophobic surfaces

Associated CINT Scientist:
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Bio-inspired and bio-compatible materials

The biomaterials synthesis capabilities will enable researchers to isolate, engineer, and integrate biological molecules with nanoscale synthetic materials and systems. Because native biological molecules are, in general, poorly suited for integration with synthetic systems, we focus upon engineering biomaterials specifically designed to function in synthetic nanosystems. Additionally, functionalization of biological molecules will be studied with respect to developing strategies for integrating living and non-living components that have a common interface. The capabilities that are available to CINT Users include:

- Isolation of genomic DNA, RNA, and plasmids from a variety of sources such as bacteria, viruses, and eukaryotic cells
- Growth and maintenance of a range of organisms (e.g., thermophiles, halophiles, etc.)
- Recombinant DNA cloning and expression in prokaryotic and eukaryotic systems
- Genetic engineering using reverse transcription, the polymerase chain reaction (PCR) and site-directed mutagenesis (SDM)
- Expression, purification, characterization, and functionalization of native and recombinant proteins
- Synthesis and functionalization of bio-compatible nanocrystal optical and magnetic tags (semiconductor and metal nanocrystals)
- Design of heterfunctional biomolecules for materials assembly
- Mammalian cell culture (nanoparticle interactions, cell/sub-cellular targeting of nanoparticles, etc.)

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Biomolecular Recognition

Nature utilizes molecular recognition for the control of protein-protein and protein-inorganic interactions that are key for control of cell-cycle processes and for the exquisite assembly of inorganic materials. We have the ability to create recognition molecules through biological means (phage display). These ligands can be used for recognition ligands in biosensors or for the hierarchical assembly of materials with emergent properties.

Nanomaterials assembly:

- Phage display with custom peptide/scFv libraries
- Advanced peptide synthesis and characterization
- Amphiphilic assemblies

Biosensor development:

- Recognition ligand generation against proteins or organisms
- Integration of ligands with devices/surfaces
- Biosensor testing

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II. CINT Experimental Capabilities: *Characterization*

Atom tracking scanning tunneling microscopy
Our atom-tracking scanning tunneling microscopes (STM) are used to study the motion of individual atoms, molecules, or clusters over crystal surfaces as a function of temperature. In atom-tracking mode the STM probe tip is "locked" onto a diffusing adsorbate using lateral, X-Y, feedback and the diffusion path is continually monitored. This mode increases the time resolution of kinetic measurements by a factor of 1000 over conventional STM imaging. Facilities that will be available include:

- Atom-tracking STM studies (selected metals, Si, Ge)
- Kinetic modeling of surface diffusion

Associated CINT Scientist:
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High Resolution Scanning Electron Microscope and Focused Ion Beam
The Nova 600 Nanolab from FEI Company combines ultrahigh resolution SEM with FIB capabilities in one machine for sample analysis, 2D and 3D machining, and prototyping. The resolution of 1.1 nm at 15 kV in secondary electron mode is further enhanced when using the STEM detector. This DualBeam™ machine also allows for electron and ion induced deposition of metals from gas source precursors (currently, Pt) with line widths of 50 nm (ion beam) and 20 nm (electron beam). An auto FIB, auto TEM, and pattern generation module is available for ion milling to provide automation of many tasks.

Technical Contact:
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Environmental Scanning Electron Microscope
The Quanta 400 FEG from FEI Company is a high resolution electron microscope that allows data collection from a variety of samples due to its ability to image at relatively high background pressures while reducing sample charging. The system is equipped with a cooling stage, solid-state STEM detector, BSE detector, and Genesis EDS.

Technical Contact:
Dr. Darrick Williams, darrick@lanl.gov, (505) 665-2081

X-ray Diffraction
The Rigaku Ultima III is a powder diffractometer that operates in a theta/2theta mode that can analyze many different type of samples (bulk powders, thin-films and liquids). The system is equipped with a standard powder stage, a thin-film stage, a small angle X-ray scattering stage (SAXS) and a Differential Scanning Calorimetry-X-ray Diffraction Stage (DSC-XRD) stage. Also here at CINT we have software to analyze bulk powders (Crystal Maker, Jade, GSAS), thin-film (diffraction, reflectivity, SAXS) and liquids that contain (Spherical, Core/Shell and Rods nanoparticles).

Technical Contact:
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Transmission Electron Microscopy
A Tecnai G(2) F30 S-Twin 300 kV transmission electron microscope made by FEI Company is available in CINT. The instrument has a resolution in TEM mode of 0.20 nm at 300 kV, but is configured to operate also at 200 kV and 100 kV with resolutions of 0.25 and 0.32 nm, respectively. The unit is equipped with scanning capability with a resolution of 0.14 nm in high-angle annular dark-field (HAADF) mode. The instrument is equipped with energy-dispersive x-ray analysis for detection of characteristic x-rays for elemental analysis, and an electron energy-loss spectrometer for characterizing composition as well as for energy-filtered imaging.

The instrument can be used for characterization of materials at the nanometer-scale, imaging small nanostructures or nano-components being integrated together, and *in situ* experimentation of nanostructure materials such as tensile testing or elevated temperature reactions.

Associated CINT Scientist:
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Optical spectroscopy
Optical spectroscopy is an essential tool for the characterization of many nanomaterials. Although these techniques are not capable of directly resolving individual nanostructures they can be used for investigating important nanoscale processes such as energy transfer and plasmonic transport. The available capabilities include:

- Optical spectroscopy, UV-Vis, Fluorescence Spectroscopy, FTIR
- Raman and Infrared Spectroscopy
- Ellipsometry
- Attenuated total reflection (ATR) spectroscopy
- Thin-film and 3-D waveguide characterization
- Silicon Photonics switching and sensing
- Light scattering
- Interferometry
- Cryogenic and magnetic fields in combination with optical spectroscopy

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Optical microscopy and single molecule spectroscopy
Advanced spectroscopic techniques can be combined with optical microscopy to provide a suite of tools for characterizing the spatially dependent properties of nanoscale materials. The available capabilities include:

- Microscopy: : light, fluorescence, and high-resolution hyper-spectral
- Single-molecule fluorescence detection, imaging and spectroscopy techniques including : confocal scanning microscopy (one- and two-photon excitation) ; wide-field, CCD camera imaging using epi-illumination or total internal reflection excitation ; single-molecule fluorescence flow cytometry ; time-correlated single-photon counting ; fluorescence correlation spectroscopy ; polarization anisotropy; single molecule tracking in two and three dimensions
- Near-field scanning optical microscopy, combined with both cw and transient absorption spectroscopy
- Low temperature optical microscopy/spectroscopy in combination with various scanning probe techniques

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Ultrafast laser spectroscopy
Ultrafast spectroscopy provides important information about the excitation and relaxation dynamics occurring in nanomaterials. A suite of ultrafast excitation and diagnostic capabilities, spanning wavelengths from the ultraviolet to the far-infrared are available for dynamic nanoscale characterization. These capabilities enable coherent quantum control experiments, as well as experiments for dynamic materials characterization. The available capabilities include:

- Femtosecond broadband transient absorption spectroscopy (infrared to ultraviolet)
- Time-resolved femtosecond photoluminescence
- Degenerate and non-degenerate four-wave mixing
- Optical pump/terahertz probe spectroscopy
- Ultrafast scanning tunneling microscopy
- Ultrafast optical characterization at photonic wavelengths (1.55 μm)
- Femtosecond pulse shaping capability with 20 fs optical pulses and electric field measurement diagnostics
- Cryogenic and magnetic field in combination with ultrafast spectroscopy

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Single-molecule manipulation, biomolecular motor mechanics and application of calibrated magnetic forces
Instrumentation for parallel application of calibrated vertical magnetic forces with simultaneous evanescent wave scattering readout of polymer length. Suitable for:

- Unzipping individual short DNA molecules to monitor protein binding, measure equilibrium association constants, and probe binding kinetics with dynamic force spectroscopy (DFS).
- Epi-illumination tethered particle motion (TPM) monitoring of single-molecule transcription with and without dynamic magnetic forces.
- Characterizing unbinding forces of any receptor-ligand system that can be set up in the magnetic microsphere / planar glass slide configuration.

Instrumentation for application of calibrated horizontal magnetic forces or application of fields using customized magnetic pole piece configurations. Suitable for:

- Calibrating magnetic forces on polymer / superparamagnetic nanoparticle composites using micromachined piconewton force sensing spring; sensitive to 300 femtograms magnetite (or equivalent sat. moment), 1 pN force sensitivity, and >= 500 nm microsphere radius.
- Laterally stretching / unzipping single molecule tethers (e.g. lambda DNA, chromatin) monitoring force-extension with cross-correlation video tracking.
- Application of forces to molecular motor / shuttle systems via attached magnetic microspheres.
- In-cell manipulation of functionalized magnetic nanoparticles.

Custom software applications for tethered particle motion (TPM) analysis, in-plane motion tracking, dynamic force spectroscopy (DFS) analysis and simulation, polymer force-extension modeling.

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Ion Beam Materials Laboratory

The core of the laboratory consists of a 3.2 MV Pelletron® tandem ion accelerator and a 200 kV ion implanter. The tandem accelerator has five beam lines with a series of experimental stations that support various research programs. The operation of IBML and its interactions with users are organized around core facilities and experimental stations. The IBML provides and operates the core facilities, while supporting the design and implementation of specific apparatus needed for experiments requested by users of the facility. This results in a facility with competencies in routine ion beam experiments and the versatility to cater to the individual researchers needs. Detailed information is available at http://www.lanl.gov/mst/ibml/. Available capabilities include:

- Materials modification and synthesis through ion implantation with various ion species (gases, transition metals and rare earth) under various temperatures
- Materials characterization using ion beam analysis techniques:
  - *Rutherford backscattering spectrometry*
  - *High energy elastic scattering spectrometry*
  - *Elastic recoil detection analysis or Forward recoil spectrometry*
  - *Nuclear reaction analysis*
  - *Particle induced X-ray emission spectroscopy*
  - *Ion channeling with a 5-axis goniometer*
- Ion beam induced radiation damage in metals, semiconductors, and insulators
- Alpha radiolysis of gases, liquids, and polymers (FTIR and RGA)
- Nuclear microprobe for ion beam microanalysis and microfabrication
- Joint target chamber for Implanter and Accelerator to conduct in situ ion implantation and ion beam analysis

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Mechanical properties from very small regions

The mechanical properties of thin films and layered materials or very small volumes of materials cannot be measured using conventional techniques. Nanoindentation methods have been developed to probe materials at depths of tens of nanometers over regions with dimensions of hundreds of nanometers. Using continuous stiffness measurement, we have the capability to measure changes in mechanical properties as a function of depth. Substrate or layering effects can also be examined. We have also measured material length scales and size effects resulting from dislocation concentrations and dislocation interactions with other structural defects. Changes in material properties resulting from impurities, second phase inclusions or engineered nanostructures can also be measured. Specific capabilities include two nanoindenters with continuous stiffness measurement up to 2 N, lateral force measurement, AFM scanning, nanopositioning, and a thermal stage.

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Variable and low temperature electronic transport

The electronic properties of nanoelectronic structures exhibit quantum mechanical and interaction effects at low temperatures and high magnetic fields. Devices designed to explore these effects can be fabricated on compound semiconductor heterostructures using standard microfabrication techniques. The primary capabilities for transport characterization of nanoelectronic devices will be a rapid turn-around ^{3}He system for 0.3 K to 300 K, and a dilution refrigerator for reaching 0.02 K. These systems will be in a 13 T wide bore magnet.

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Atomic force microscopy, near field and fluorescence imaging

Full imaging and characterization of biological interfaces and electronic materials and devices are available. On-going projects include membranes and model lipid systems, and defects in wide bandgap semiconductors. The facility will include atomic force microscopy in ambient and fluid environments, in tandem with far-field fluorescence imaging and apertureless near-field imaging. Facilities that will be available include:

- Atomic force microscopy: topography, phase imaging
- Atomic force combined with fluorescence microscopy, including apertureless near-field techniques
- Conducting tip atomic force microscopy: scanning capacitance, scanning Kelvin force, piezoelectric force, and scanning current-voltage microscopy

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Interfacial force microscopy
The Interfacial Force Microscope (IFM) is a unique, Sandia-developed scanning force-probe technique featuring a mechanically stable, self-balancing force sensor, which has the capability to quantitatively measure normal and lateral interfacial forces at the nanoscale. Current interests for IFM applications include: (1) studies of the fundamental mechanisms underlying molecular-level friction for functionalized surfaces; (2) studies of the nanomechanical properties of self-assembled films, interphase materials and solid surfaces, including molecular films, polymers and metals; and (3) studies of the fundamental aspects of charge transfer in various systems under non-contact, contact and under applied stress. The capabilities that are currently available include:

- IFM instrumentation with broad facilities for tip and sample preparation and analysis, molecular self assembly and environmental control;
- Controlled Imaging capabilities for quantitative analysis of, e.g., morphology, complex-modulus mapping, conductance, friction, etc.
- Control of tip material, size, shape and chemical functionality;
- Considerable experience in data analysis to obtain fundamental materials properties.

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Low energy electron microscopy (LEEM)
The low energy electron microscope (LEEM) is a unique and versatile surface microscope that can be used to view dynamic processes on surfaces in real time with a spatial resolution of 7-8 nm and a depth resolution of one atomic layer. The LEEM provides high image contrast between regions on a surface with different atomic structures or chemical compositions. Because it is a non-scanning microscope, dynamic processes can be observed with a time resolution limited only by the video recording rate of the image acquisition system. Current interests for LEEM applications include: 1) studies of the fundamental mechanisms underlying self-assembly and pattern formation on solid surfaces, 2) studies of the evolution of surface morphology including thermal smoothing mechanisms, 3) studies of the fundamental aspects surface phase transitions and surface chemical reactions, 4) studies of doping distributions and surface oxide charging effects in microelectronic device structures, and 5) the development of LEEM-IV analysis to obtain 3-D compositional maps of the surface and near surface regions of crystalline solids.

Specific capabilities of the LEEM include:

- Ultra-high vacuum ($<1\text{x}10^{-10}$ Torr) in main chamber
- Sample cleaning by ion bombardment and thermal annealing
- Surface characterization by Auger Electron Spectroscopy
- Images can be recorded with the sample at temperatures from 200 K to 1800 K
- Images can be recorded with a flux of atoms or molecules impinging on the surface

Associated CINT Scientist:
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Magnetic Resonance Force Microscopy
The Magnetic Resonance Force Microscope (MRFM) is a unique instrument that allows 3D microscopic imaging of magnetic entities, such as magnetic clusters, surfaces, and buried interfaces. MRFM is based on a mechanical detection of magnetic resonance signals. In conjunction with the AFM-like surface resolution it enables spatial imaging, similar to the conventional Magnetic Resonance Imaging (MRI) but with much higher accuracy.

We are capable to carry out the measurements in the fields up to 6T and temperatures down to 4K with the resolution of ~ 10^3 electron spins. Facilities that will be available include:

- MRFM studies
- Ferromagnetic Resonance Force Microscopy (FMRFM) studies

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III. CINT Theory and Simulation Capabilities

The advances of computing technologies and modeling approaches have enabled detailed studies of collective and cooperative materials phenomena at various length scales. However, it is well recognized that fundamental understanding of the behaviors of nanostructured materials will not be addressed by simple extensions of current theoretical methods that are focused on either atomic or macro scales, but will require bridging the gap between these scales with new concepts, new modeling frameworks and new simulation schemes. The Theory and Simulation thrust area supports CINT Users by providing expertise in a number of fields including theory, predictive capability development, interpretation and design of experiments, multiscale material modeling, and large scale computing. The capabilities that are available to CINT Users include:

- *Simulation tools for computational materials science*
  - LAMMPS: a parallel molecular dynamics code for classical atomistic and coarse grained level simulations
    POC: Dr. Mark J. Stevens, msteve@sandia.gov, (505) 844-1937
  - TRAMONTO: a parallel, classical density functional theory code for atomic and polymeric fluids
    POC: Dr. Amalie L. Frischknecht, alfrisc@sandia.gov, (505) 284-8585
  - Socorro: a parallel quantum density functional theory code for investigating the electronic structure and predicting ground state and dynamical properties of systems containing up to 1000 atoms
    POC: Dr. Normand A. Modine, namodin@sandia.gov, (505) 844-8412
  - A variety of tools for visualization and analysis
    POC: Dr. Alexander Balatsky, avb@lanl.gov, (505) 665-0077

- *Simulations using atomistic or coarse-grained models for studying nanoparticles, biomolecules and polymers*
  - Techniques: molecular dynamics simulations
  - Atomistic simulations of interactions between coated nanoparticles
  - Simulation of lipid bilayer systems
  - Simulation of charged polymers
  - Molecular simulation of interfacial phenomena
    POC: Dr. Mark J. Stevens, msteve@sandia.gov, (505) 844-1937

- *First-principles quantum and quantum/classical modeling of the effects of surfaces, interfaces, and defects on chemical, electronic, and mechanical dynamics*
  - Techniques: Kohn-Sham density functional theory,
  - Quantum Mechanics / Molecular Mechanics (QM/MM),
  - Molecular dynamics
    POC: Dr. Normand A. Modine, namodin@sandia.gov, (505) 844-8412

- *Theory and simulation of complex fluids including polymeric, colloidal, and biological materials*
  - Techniques: molecular theory including classical density functional theory for fluids and self-consistent field theory; molecular dynamics simulations
    POC: Dr. Amalie L. Frischknecht, alfrisc@sandia.gov, (505) 284-8585

- *Large-scale molecular dynamics simulations of biomolecules and molecular motors*
  - Techniques: molecular dynamics simulations
    POC: Dr. Sergei Tretiak, serg@lanl.gov, (505) 662-0466

- *Computational models for complex fluids, polymer melts and networks, self-assembled monolayers, and granular materials*
  - Techniques: molecular dynamics and Monte Carlo simulations
    POC: Dr. Gary S. Grest, gsgrest@sandia.gov, (505) 844-3261

- *Effects of impurities, defects, surfaces, interfaces, and other inhomogeneities on local electronic properties, and how they help control functionality in nanoscale electronic devices*
  - Theory of single impurities in high temperature superconductors
  - Theory of single spin dynamics on metallic surfaces
  - Theory of electron tunneling through quantum dots with electron-electron correlation, single molecules with electron-vibration coupling
  - Theory of electron transport in unconventional (ferromagnetic, superconducting, organic) tunnel junctions
    POC: Dr. Alexander Balatsky, avb@lanl.gov, (505) 665-0077

- *Theory and models of multi-particle excitations and energy/charge transport phenomena in semiconductor nanocrystals and their assemblies*
  - Techniques: density functional theory and solid-state (e.g. tight-binding) approaches
    POC: Dr. Sergei Tretiak, serg@lanl.gov, (505) 662-0466

- *Quantum-chemical simulation of photoinduced adiabatic and non-adiabatic excited state dynamics in conducting polymers and (bio)organic chromophores*
  - CEO: LANL-developed parallel molecular dynamics code based on semiempirical approaches
  - TURBOMOLE: ab initio molecular dynamics package
  - Reduced Hamiltonian models for treating state crossings and conical intersections
    POC: Dr. Sergei Tretiak, serg@lanl.gov, (505) 662-0466

- *Computational modeling of nonlinear optical responses (e.g. two-photon absorption, second and third harmonic generations) in organic and organo-metallic chromophores*
  - Techniques: quasi-particle density matrix response formalism in combination with time-dependent density functional theory
    POC: Dr. Sergei Tretiak, serg@lanl.gov, (505) 662-0466

- *Theory and models for nano-electro-mechanical and spin systems out of equilibrium, such as single electron transistors coupled to mechanical degrees of freedom*
  - Techniques: field theory Keldysh formalism for non-equilibrium systems, approximation techniques based on separation of time scales, impurity-averaged perturbation theory for studying disorder effects.
    POC: Dr. Alexander Balatsky, avb@lanl.gov, (505) 665-0077

- *Theory of transport and optical properties of semiconductor nanostructures and conjugated organic materials; properties of devices fabricated from these materials*
  - Techniques: electronic structure, quantum non-equilibrium models, and mesoscale device models
    POC: Dr. Darryl L. Smith, dsmith@lanl.gov, (505) 667-2056
    POC: Dr. Alexander V. Balatsky, avb@lanl.gov, (505) 665-0077

- *Noise spectroscopy, single molecule spectroscopy, single spin detection, inelastic tunneling spectroscopy, strongly correlated electrons, scanning probes microscopy, DNA nanoelectronics*
  - Techniques: Green's functions, nonequilibrium kinetics, electronic transport
    POC: Dr. Alexander V. Balatsky, avb@lanl.gov, (505) 665-0077

- *Theory of quantum dynamics of coupled systems, including inelastic tunneling dynamics and fast optical probes of correlated systems*
  - Techniques: exact diagonalization, Lanczos, and numerical quantum dynamics in a large many-body Hilbert space
    POC: Dr. Stuart Trugman, sat@lanl.gov, (505) 665-1167

- *Theory and modeling of ac transport in nano-devices; single-spin measurement; spin qubits in solids*
  POC: Dr. Alexander Balatsky, avb@lanl.gov, (505) 665-0077

For general information, contact:
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IV. Other SNL/LANL National User Facilities

Los Alamos Neutron Science Center – LANSCE
For detailed information see: http://lansce.lanl.gov/index_ext.htm

National High Magnetic Field Laboratory – NHMFL
For detailed information see: http://www.lanl.gov/mst/nhmfl/

Combustion Research Facility – CRF
For detailed information see: http://www.ca.sandia.gov/CRF/